

chain nodes :

11 13

ring nodes :

1 2 3 4 5 6 7 8 9 10

chain bonds :

1-11 11-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10

exact/norm bonds :

1-11 4-7 5-10 7-8 8-9 9-10 11-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
13:Atom

10/702,295

=> d his

(FILE 'HOME' ENTERED AT 11:51:27 ON 08 MAR 2006)

FILE 'REGISTRY' ENTERED AT 11:51:32 ON 08 MAR 2006

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 STRUCTURE UPLOADED

L4 1 S L3

FILE 'CAPLUS' ENTERED AT 11:52:52 ON 08 MAR 2006

L5 476 S BARBOSA J?/AU

L6 199 S PITTS W?/AU

L7 6519 S GUO J?/AU

L8 9 S L5 AND L6 AND L7

L9 4 S L8 AND PATENT/DT

L10 2 S HETEROCYCLIC/TI AND L9

FILE 'REGISTRY' ENTERED AT 11:55:54 ON 08 MAR 2006

L11 11 S L3 SSS FUL

FILE 'CAPLUS' ENTERED AT 11:57:16 ON 08 MAR 2006

L12 2 S L11

=> d ibib abs hitstr total

10/702,295

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:244464 CAPLUS

DOCUMENT NUMBER: 142:463684

TITLE: Fused pyrimidine based inhibitors of phosphodiesterase 7 (PDE7): synthesis and initial structure-activity relationships

AUTHOR(S): Kempson, James; Pitts, William J.; Barbosa, Joseph; Guo, Junqing; Omotoso, Omonike; Watson, Andrew; Stebbins, Karen; Starling, Gary C.; Dodd, John H.; Barrish, Joel C.; Felix, Raymond; Fischer, Karl

CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543-4000, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(7), 1829-1833

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of fused pyrimidine based inhibitors of PDE7 have been derived from an earlier screening lead. The synthesis, structure-activity relationships (SAR) and selectivity against several other PDE family members are described.

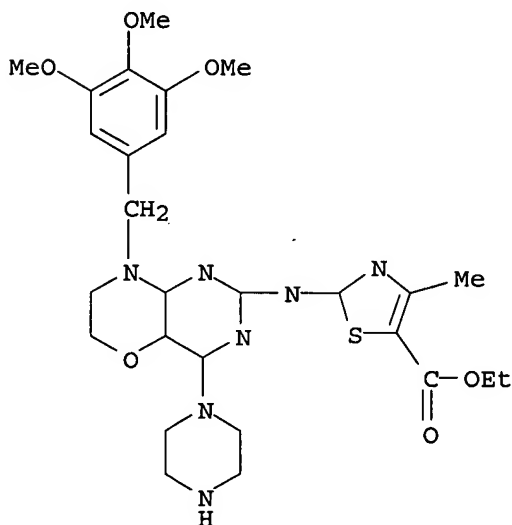
IT 851787-09-2P 851787-10-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and structure-activity relationships of fused pyrimidine-based inhibitors of phosphodiesterase 7)

RN 851787-09-2 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[7,8-dihydro-4-(1-piperazinyl)-8-[(3,4,5-trimethoxyphenyl)methyl]-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

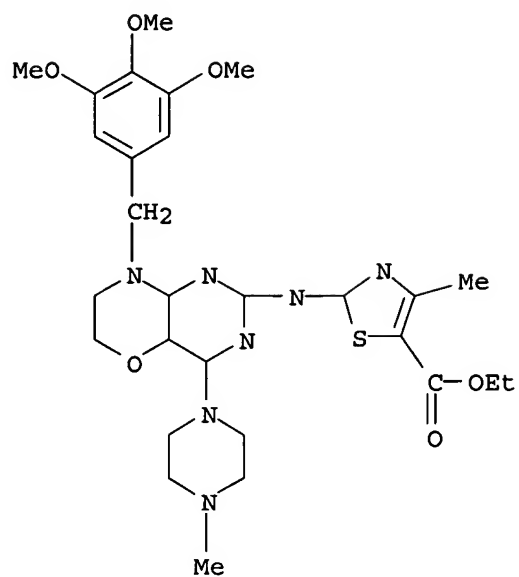


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 851787-10-5 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[7,8-dihydro-4-(4-methyl-1-piperazinyl)-8-[(3,4,5-trimethoxyphenyl)methyl]-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

10/702,295



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/702,295

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:430699 CAPLUS

DOCUMENT NUMBER: 141:7128

TITLE: Preparation of fused heterocycles, in particular fused pyrimidines, for use in treatment of leukocyte activation-associated disorders

INVENTOR(S): Barbosa, Joseph; Pitts, William J.; Guo, Junqing

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 157 pp.

CODEN: PIXXD2

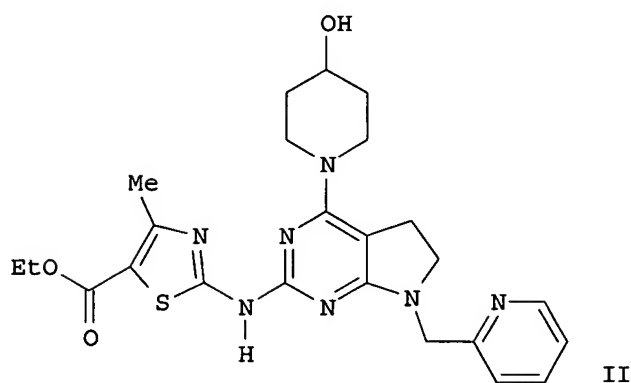
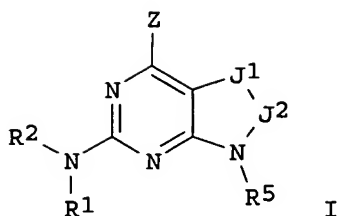
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004043367	A2	20040527	WO 2003-US35321	20031106
WO 2004043367	A3	20041014		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2004142945	A1	20040722	US 2003-702295	20031106
PRIORITY APPLN. INFO.:			US 2002-424250P	P 20021106
OTHER SOURCE(S):	MARPAT 141:7128			
GI				



AB The title compds. [I; R1 = H, alkyl; R2 = (un)substituted heteroaryl, heterocycle, aryl, aryl fused to heteroaryl or heterocycle with proviso; R5 = H, CN, (un)substituted alk(en/yn)yl, cycloalkyl, heterocyclyl, CO₂H and derivs., etc.; Z = NH₂ and derivs., OH and derivs., SH and derivs., haloalkyl, halo; J1 = O, S, SO, SO₂, (un)substituted C1-3 alkylene; J2 = CO, (un)substituted C1-3 alkylene; provided that J1 and J2 taken together are not > C4; their enantiomers, diastereomers, and pharmaceutically acceptable salts, prodrugs, and solvates] were prepared as inhibitors of T-cell proliferation for treating leukocyte activation-associated disorders. E.g., a multi-step synthesis of II is given. Pharmaceutical composition comprising the compound I is claimed.

IT **695182-40-2P**, 2-[[8-[4-(Methanesulfonyl)benzyl]-4-(3-oxopiperazin-1-yl)-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methylthiazole-5-carboxylic acid ethyl ester **695182-48-0P**, 4-Methyl-2-[[4-(morpholin-4-yl)-8-(3,4,5-trimethoxybenzyl)-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]thiazole-5-carboxylic acid ethyl ester **695182-50-4P**, 4-Methyl-2-[[4-(morpholin-4-yl)-8-(4-sulfamoylbenzyl)-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]thiazole-5-carboxylic acid ethyl ester **695182-52-6P**, 2-[[4-(4-Hydroxypiperidin-1-yl)-8-(4-sulfamoylbenzyl)-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methylthiazole-5-carboxylic acid ethyl ester **695182-53-7P**, 4-Methyl-2-[[4-(3-oxopiperazin-1-yl)-8-(4-sulfamoylbenzyl)-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]thiazole-5-carboxylic acid ethyl ester **695182-54-8P**, 2-[[8-[4-(Methanesulfonyl)benzyl]-4-(morpholin-4-yl)-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methylthiazole-5-carboxylic acid ethyl ester **695182-55-9P**, 2-[[4-(4-Hydroxypiperidin-1-yl)-8-[4-(methanesulfonyl)benzyl]-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methylthiazole-5-carboxylic acid ethyl ester
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

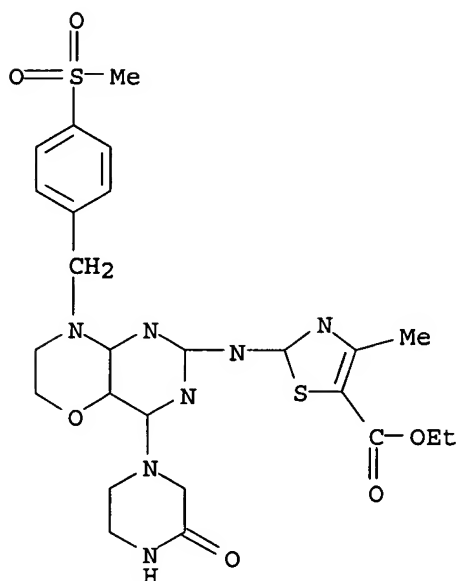
10/702,295

(Uses)

(drug candidate; preparation of fused heterocycles, in particular fused pyrimidines, for use in treatment of leukocyte activation-associated disorders)

RN 695182-40-2 CAPLUS

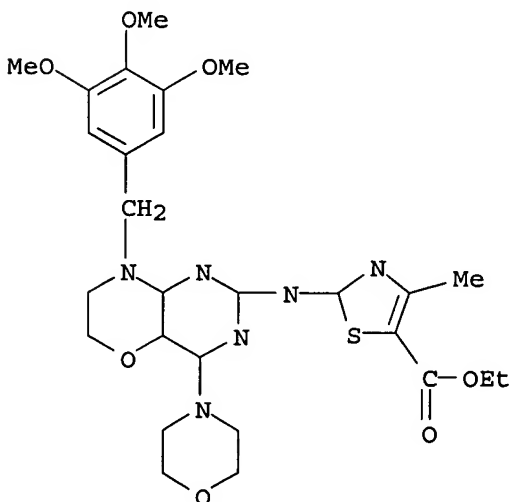
CN 5-Thiazolecarboxylic acid, 2-[[[7,8-dihydro-8-[[4-(methylsulfonyl)phenyl]methyl]-4-(3-oxo-1-piperazinyl)-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 695182-48-0 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[[7,8-dihydro-4-(4-morpholinyl)-8-[(3,4,5-trimethoxyphenyl)methyl]-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

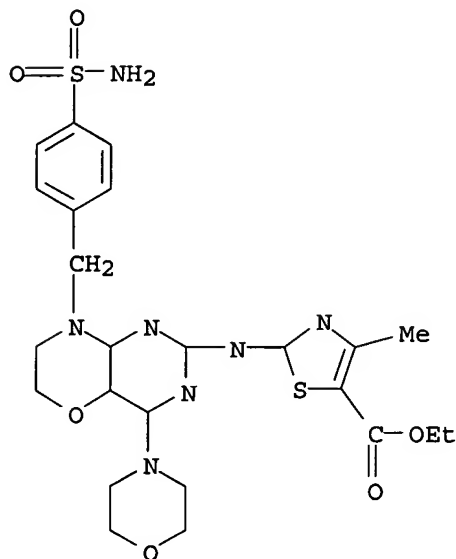


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ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 695182-50-4 CAPLUS

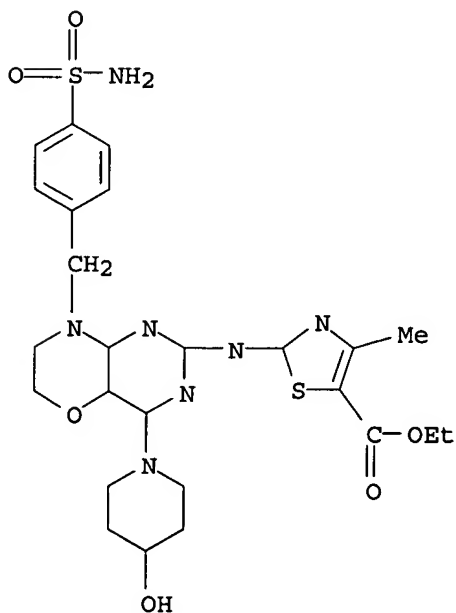
CN 5-Thiazolecarboxylic acid, 2-[[8-[[4-(aminosulfonyl)phenyl]methyl]-7,8-dihydro-4-(4-morpholinyl)-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 695182-52-6 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[8-[[4-(aminosulfonyl)phenyl]methyl]-7,8-dihydro-4-(4-hydroxy-1-piperidiny)l)-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

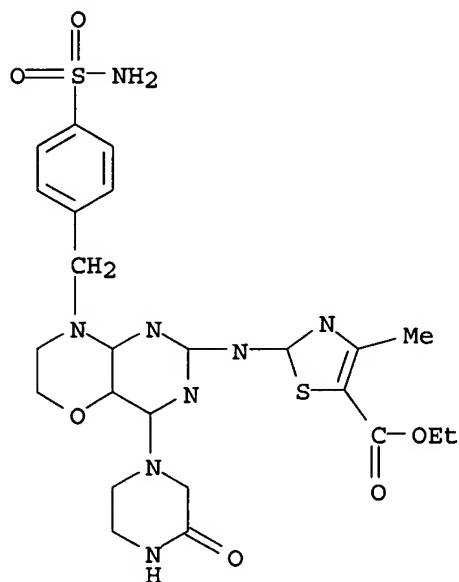


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ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 695182-53-7 CAPLUS

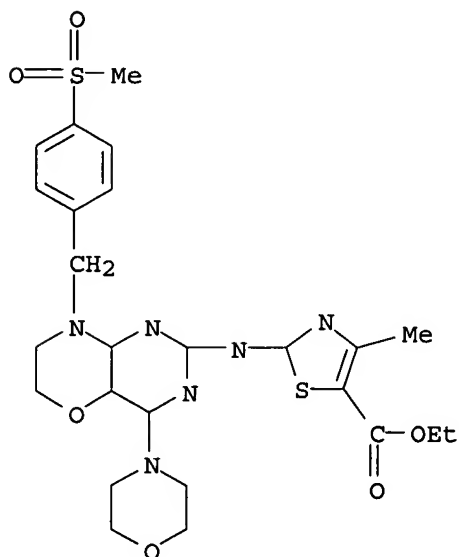
CN 5-Thiazolecarboxylic acid, 2-[[8-[[4-(aminosulfonyl)phenyl]methyl]-7,8-dihydro-4-(3-oxo-1-piperazinyl)-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 695182-54-8 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[7,8-dihydro-8-[[4-(methylsulfonyl)phenyl]methyl]-4-(4-morpholinyl)-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

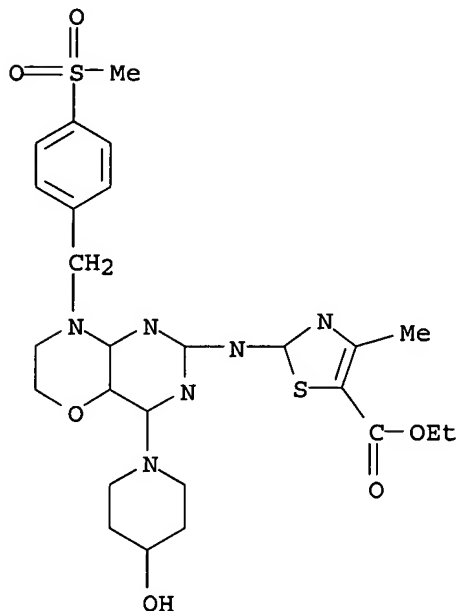


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

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RN 695182-55-9 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[7,8-dihydro-4-(4-hydroxy-1-piperidinyl)-8-[[4-(methanesulfonyl)phenyl]methyl]-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

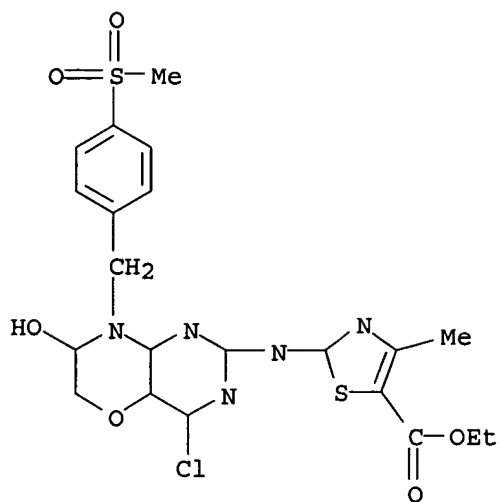
IT 695182-44-6P, 2-[[4-Chloro-7-hydroxy-8-[4-(methanesulfonyl)benzyl]-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methylthiazole-5-carboxylic acid ethyl ester 695182-46-8P, 2-[[4-Chloro-8-[4-(methanesulfonyl)benzyl]-6,7-dihydro-8H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methylthiazole-5-carboxylic acid ethyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of fused heterocycles, in particular fused pyrimidines, for use in treatment of leukocyte activation-associated disorders)

RN 695182-44-6 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[4-chloro-7,8-dihydro-7-hydroxy-8-[[4-(methanesulfonyl)phenyl]methyl]-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

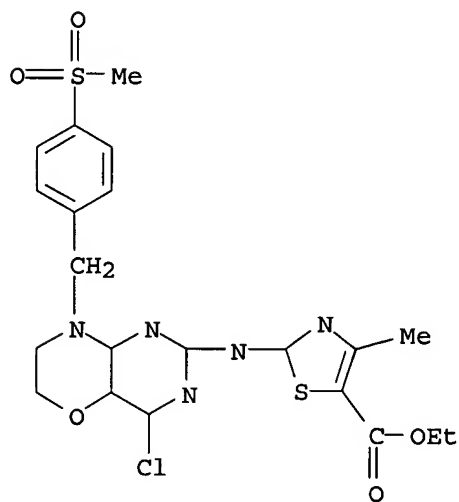
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ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 695182-46-8 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[4-chloro-7,8-dihydro-8-[[4-(methylsulfonyl)phenyl]methyl]-6H-pyrimido[5,4-b][1,4]oxazin-2-yl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

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